Chapter 20
Sensitivity Analyses of Initial Compositions and Cross Sections for Activation Products of In-Core Structure Materials

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Abstract Sensitivity analyses of initial compositions and cross sections were conducted to quantitatively clarify the source elements and the nuclear reactions dominating the generation of activation products. In these analyses, the ORIGEN2.2 code was used with ORLIBJ40, a set of the cross-section libraries based on JENDL-4.0. Analyses were conducted for the activations of cladding tubes, end plugs, and spacers of fuel assemblies and channel boxes in BWR that are composed of zirconium alloy, stainless steel, and nickel-chromium-based alloy. From about 50 representative radioactive nuclides, several nuclides were selected as the targets of sensitivity analyses for the aspect of their large concentrations in the target materials.

The results of sensitivity coefficients clarified the source elements and the nuclear reactions dominating the generation of activation products even for the nuclides generated through complicated pathways. These results could be utilized to select the objectives of the impurity elements for measurements and of nuclear data for the improvement of accuracy. These results will contribute to improvements in the accuracy of numerical evaluations of activation product concentrations.

Keywords Activation products • Burn-up calculation • INCONEL alloy • ORIGEN2.2 • ORLIBJ40 • Sensitivity study • Stainless steel • Zircaloy

20.1 Introduction

In the research on the back-end of nuclear cycles, improvement of the accuracy of predicting concentrations of activation products is important for various evaluations. Providing the accurate initial compositions and nuclear data leading to the generation of activation products is necessary for accurate predictions of

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K. Nakajima (ed.), *Nuclear Back-end and Transmutation Technology for Waste Disposal*, DOI 10.1007/978-4-431-55111-9_20

concentrations of the activation products. An effective first step to achieving this is to identify the dominant generation pathways of activation products. Sensitivity analyses of initial compositions and cross sections for activation products, which involve understanding the effects of initial compositions and cross sections on the concentrations of the target activation products, are powerful methods for quantitatively investigating the generation pathways. Thus, in the present study, sensitivity analyses focusing on the generation pathways for activation products were conducted.

The ORIGEN2.2 [1] code was used in the analyses; this code has been widely used for evaluating the concentrations of activation products. The one-group cross sections made with the appropriate neutron spectrum are required for the accuracy of the ORIGEN2.2 calculation. With respect to the activations of in-core structure materials, the existing ORIGEN2.2 cross-section libraries made with the in-core neutron spectrum are available. Thus, the target of the analyses in the present study is the activation of such in-core structure materials.

This chapter presents the method, calculation conditions, and results of the sensitivity analyses of initial compositions and cross sections for activation products in the materials of in-core structures, such as zirconium alloy, stainless steel, and nickel-chromium-based alloy. The results of the sensitivity analyses identify the elements and the nuclear reactions leading to the generation of activation products. These results will be effective in improving the accuracy of numerical evaluations of the concentrations of activation products.

20.2 Method of Calculating Sensitivity Coefficients

A sensitivity coefficient is defined as the ratio of the variation in concentration of the target activation product to the variation in the initial composition or cross section. The sensitivity coefficient of the initial composition and cross section is expressed by the following equations, respectively:

$$S = \frac{\Delta W / W_0}{\Delta X / X_0} \tag{20.1}$$

$$S = \frac{\Delta W / W_0}{\Delta \sigma / \sigma_0} \tag{20.2}$$

W_0: Concentration of the target activation product under normal condition
$\Delta W (= W' - W_0)$: Variation in concentration of the target activation product
X_0: Initial concentration of the element in the material under normal condition
$\Delta X (= X' - X_0)$: Variation in initial concentration of the element in the material
σ_0: Cross section under normal condition
$\Delta \sigma (= \sigma' - \sigma_0)$: Variation in cross section

For the calculation of concentration of activation products, ORIGEN2.2 was used with ORLIBJ40 [2], which is a set of the one-group cross-section libraries based on JENDL-4.0 [3]. The sensitivity coefficients are evaluated by executing two different burn-up calculations under normal condition and under composition-changed or cross-section-changed condition. In the former, the ORIGEN2.2 input files are changed; in the latter, the cross-section library files are changed. Utility programs to evaluate the sensitivity coefficients were prepared and used in these analyses.

20.3 Sensitivity Analyses

20.3.1 Analyses Conditions

As stated in Sect. 20.1, activations of in-core structure materials, such as cladding tubes, end plugs, and spacers of fuel assemblies and channel boxes, were investigated in this study. The materials of the in-core structures of PWR and BWR are shown in Table 20.1. The compositions of Zircaloy-2, Zircaloy-4, SUS304 stainless steel, and INCONEL alloy 718 are shown in Table 20.2. In Table 20.2, the average value of the upper and lower limits of the standard specification was applied to the calculation condition for additive elements and the upper limit was applied for impurity elements. The effect of impurity elements that are not specified in the standard are investigated in Sect. 20.3.4.

Typical conditions of BWR were assumed for the cross-section libraries and the irradiation condition, because the difference between the conditions of PWR and BWR is not so significant for the purpose of this study, which is clarifying the dominant generation pathways of activation products.

The cross-section libraries used in these analyses (Table 20.3) were chosen to correspond to the condition of the void ratio in the axial direction. A library made with an average void ratio (40 %) was applied to cladding tubes, spacers, and channel boxes for which the void ratio varies from 0 % to 70 %.

A BWR typical irradiation history consists of four cycles of irradiation of about 377 days with constant flux and 90 days of cooling time in the intervals of irradiation (Fig. 20.1). Considering the period for processing of radioactive wastes,

Table 20.1 Materials of in-core structure

	BWR	PWR
Cladding tube	Zircaloy-2	Zircaloy-4
Top end plug	SUS304	←
Bottom end plug	SUS304	←
Spacer	Plate: Zircaloy-2	Zircaloy-4 or
	Spring: INCONEL alloy 718	INCONEL alloy 718
Channel box	Zircaloy-4	–

Table 20.2 Compositions of materials

	Specification (wt%)			Value in analysis (wt%)
(a) Zircaloy-2 (JIS H 4751)				
H	0.0025	Max.		0.0025
B	0.00005	Max.		0.00005
C	0.027	Max.		0.027
N	0.008	Max.		0.008
Mg	0.002	Max.		0.002
Al	0.0075	Max.		0.0075
Si	0.012	Max.		0.012
Ca	0.003	Max.		0.003
Ti	0.005	Max.		0.005
Cr	0.05	–	0.15	0.10
Mn	0.005	Max.		0.005
Fe	0.07	–	0.20	0.135
Co	0.002	Max.		0.002
Ni	0.03	–	0.08	0.055
Cu	0.005	Max.		0.005
Zr		Balance		98.1456
Nb	0.01	Max.		0.01
Mo	0.005	Max.		0.005
Cd	0.00005	Max.		0.00005
Sn	1.20	–	1.70	1.45
Hf	0.01	Max.		0.01
W	0.01	Max.		0.01
U	0.00035	Max.		0.00035
(b) Zircaloy-4 (JIS H 4751)				
H	0.0025	Max.		0.0025
B	0.00005	Max.		0.00005
C	0.027	Max.		0.027
N	0.008	Max.		0.008
Mg	0.002	Max.		0.002
Al	0.0075	Max.		0.0075
Si	0.012	Max.		0.012
Ca	0.003	Max.		0.003
Ti	0.005	Max.		0.005
Cr	0.07	–	0.13	0.10
Mn	0.005	Max.		0.005
Fe	0.18	–	0.24	0.21
Co	0.002	Max.		0.002
Ni	0.007	Max.		0.007
Cu	0.005	Max.		0.005
Zr		Balance		98.1186
Nb	0.01	Max.		0.01

(continued)

Table 20.2 (continued)

	Specification (wt%)			Value in analysis (wt%)
Mo	0.005	Max.		0.005
Cd	0.00005	Max.		0.00005
Sn	1.20	–	1.70	1.45
Hf	0.01	Max.		0.01
W	0.01	Max.		0.01
U	0.00035	Max.		0.00035
(c) SUS304 stainless steel (JIS G 4303)				
C	0.08	Max.		0.08
Si	1.00	Max.		1.00
P	0.045	Max.		0.05
S	0.030	Max.		0.03
Cr	18.00	–	20.00	19.00
Mn	2.00	Max.		2.00
Fe		Balance		68.595
Ni	8.00	–	10.50	9.25
(d) INCONEL alloy 718 (UNS N07718)				
B	0.006	Max.		0.006
C	0.08	Max.		0.08
Al	0.20	–	0.80	0.50
Si	0.35	Max.		0.35
P	0.015	Max.		0.015
S	0.015	Max.		0.015
Ti	0.65	–	1.15	0.90
Cr	17.00	–	21.00	19.00
Mn	0.35	Max.		0.35
Fe		Balance		16.809
Co	1.00	Max.		1.00
Ni	50.00	–	55.00	52.50
Cu	0.3	Max.		0.30
Nb	4.75	–	5.50	5.125
Mo	2.80	–	3.30	3.05

Table 20.3 Cross-section libraries

	Specification in cross-section library
Cladding tubes, spacers, channel boxes	BWR STEP-III, void ratio 40 %
Top-end-plugs	BWR STEP-III, void ratio 70 %
Bottom-end-plugs	BWR STEP-III, void ratio 0 %

10 years of cooling time after irradiation was assumed in these analyses. The flux intensities at the center, top, and bottom in the axial direction are shown in Table 20.4. The flux intensity at the center corresponds to the average power in typical BWR fuel assemblies. The flux intensities at the top and bottom were

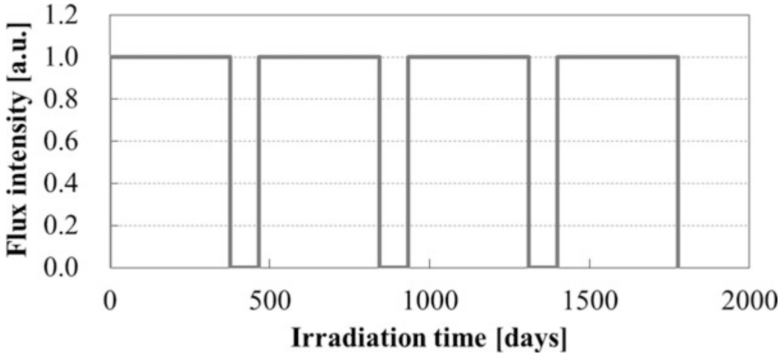

Fig. 20.1 Irradiation history

Table 20.4 Flux intensity at center, top, and bottom in axial direction

	Flux intensity (1/cm^{2}s)
Center	1.994E + 14
Top and bottom	9.970E + 12

determined to be 5 % of that at the center, based on flux distribution evaluated by the one-dimensional neutron diffusion calculation.

20.3.2 Target Nuclides of Sensitivity Analyses

The representative radioactive nuclides in this study (Table 20.5) include not only the important nuclides for various evaluations of radioactive wastes but also the nuclides whose concentrations have been measured in the past, which will be useful for the validation of numerical evaluations.

Target nuclides of sensitivity analyses were selected on the basis of two criteria. The first was that the concentrations of activation products be larger than or comparable to the concentration of fission products generated from impurity uranium in the materials. The contents of impurity uranium in Zircaloy-2 and SUS304 stainless steel were 0.00035 wt% and 0.0001 wt% [5], respectively. This value in INCONEL alloy is unknown. The second criterion was that the concentrations of activation products be comparatively large. In these analyses, activation products with concentrations more than 1×10^{-9} g/t were chosen.

The concentrations of activation products larger than 1×10^{-9} g/t and fission products generated from impurity uranium are shown in Table 20.6. The fission products were calculated under the condition that the initial composition contains only the uranium impurity. Table 20.6 also shows the selected target nuclides that satisfy the foregoing criterion: 17 nuclides in Zircaloy-2 and Zircaloy-4, 8 nuclides in SUS304 stainless steel, and 16 nuclides in INCONEL alloy were selected as the target nuclides of sensitivity analyses.

Table 20.5 Representative radioactive nuclides[a,b]

No.	Nuclide	Half-life		No.	Nuclide	Half-life		No.	Nuclide	Half-life	
1	H-3	12.3	years	21	Se-79	377.0	E3 years	41	Cs-137	30.1	years
2	Be-10	1.5	E6 years	22	Rb-87	48.1	E9 years	42	Ba-133	10.5	years
3	C-14	5.7	E3 years	23	Sr-90	28.8	years	43	Sn-126	198.0	E3 years
4	Na-22	2.6	years	24	Nb-94	20.3	E3 years	44	Sb-124	60.2	days
5	Si-32	153.0	years	25	Nb-95	35.0	days	45	Sb-125	2.8	years
6	S-35	87.5	days	26	Mo-93	4.0	E3 years	46	Ce-141	32.5	days
7	Cl-36	301.0	E3 years	27	Mo-99	2.7	days	47	Ce-144	284.9	days
8	K-40	1.2	E9 years	28	Tc-99	211.1	E3 years	48	Eu-152	13.5	years
9	Sc-46	83.8	days	29	Tc-99m	6.0	hours	49	Eu-154	8.6	years
10	Ca-41	102.0	E3 years	30	Zr-93	1.5	E6 years	50	Eu-155	4.8	years
11	Cr-51	27.7	days	31	Zr-95	64.0	days	51	Gd-153	240.4	days
12	Mn-54	312.1	days	32	Ru-103	39.3	days	52	Ho-166m	1.2	E3 years
13	Fe-55	2.7	years	33	Ru-106	1.0	years	53	Hf-181	42.4	days
14	Fe-59	44.5	days	34	Ag-108m	438.0	years	54	Au-199	3.1	days
15	Co-57	271.7	days[c]	35	Ag-110m	249.8	days				
16	Co-58	70.9	days	36	I-129	15.7	E6 years				
17	Co-60	5.3	years	37	Cd-113m	14.1	years				
18	Ni-59	76.0	E3 years	38	I-131	8.0	days				
19	Ni-63	100.1	years	39	Cs-134	2.1	years				
20	Zn-65	244.1	days	40	Cs-135	2.3	E6 years				

[a]Half-life is referred to ORLIBJ40 decay library
[b]E3 years = 10^3 years, E6 years = 10^6 years
[c]Half-life of Co-57 is not contained in ORLIBJ40, so it is referred to [4]

Table 20.6 Concentration of activation products and fission products

Nuclide	Concentration of activation products (g/t)		Concentration of fission products (g/t)	Comparison (%)	Target nuclide
	①Zry-2	②Zry-4	③	③/(①+③)	
(a) Zircaloy-2 and Zircaloy-4					
Zr-93	2.0E + 02	2.0E + 02	1.2E-03	0	○
Ni-59	3.7E + 00	4.7E-01	–	–	○
Ni-63	6.6E-01	8.9E-02	–	–	○
Co-60	5.1E-01	5.1E-01	–	–	○
C-14	4.0E-01	4.0E-01	–	–	○
Nb-94	3.0E-01	3.0E-01	3.2E-09	0	○
Sb-125	2.5E-01	2.5E-01	1.5E-06	0	○
Ca-41	3.0E-02	3.0E-02	–	–	○
K-40	2.2E-02	2.2E-02	–	–	○
Fe-55	2.1E-02	3.2E-02	–	–	○
Tc-99	9.1E-03	9.1E-03	1.7E-03	16	○
Mo-93	8.9E-03	8.9E-03	3.5E-14	0	○
Be-10	4.0E-05	4.0E-05	2.2E-08	0	○
Sr-90	2.3E-05	2.3E-05	6.0E-04	96	–
Mn-54	3.9E-06	6.1E-06	–	–	○
Ag-108m	3.3E-07	3.3E-07	5.6E-12	0	○
Rb-87	1.1E-07	1.1E-07	3.7E-04	100	–
H-3	3.0E-08	3.0E-08	5.8E-08	66	○
I-129	6.4E-09	6.4E-09	3.9E-04	100	–
Zn-65	2.8E-09	2.8E-09	–	–	○
(b) SUS304 stainless steel					
Nuclide	Concentration of activation products (g/t)		Concentration of fission products (g/t)	Comparison (%)	Target nuclide
	①Bottom	②Top	③	③/(①+③)	
Ni-59	4.8E + 01	2.6E + 01	–	–	○
Ni-63	7.7E + 00	4.1E + 00	–	–	○
Fe-55	7.0E-01	3.9E-01	–	–	○
Co-60	5.3E-03	5.0E-03	–	–	○
Mn-54	9.9E-05	9.9E-05	–	–	○
Be-10	5.7E-06	5.7E-06	2.0E-10	0	○
C-14	3.2E-06	2.3E-06	–	–	○
Cl-36	1.6E-06	4.4E-07	–	–	○

(continued)

Table 20.6 (continued)

Nuclide	Concentration of activation products (g/t)		Concentration of fission products (g/t)	Comparison (%)	Target nuclide
	①Zry-2	②Zry-4	③	③/(①+③)	
(c) INCONEL alloy 718					
Nuclide	Concentration of activation products (g/t)				Target nuclide
Ni-59	3.5E + 03				○
Ni-63	6.2E + 02				○
Co-60	2.6E + 02				○
Nb-94	1.6E + 02				○
Mo-93	5.4E + 00				○
Tc-99	5.4E + 00				○
Fe-55	3.4E + 00				○
Zr-93	1.3E-01				○
Mn-54	4.8E-04				○
Be-10	2.8E-04				○
Cl-36	1.7E-04				○
C-14	5.4E-05				○
Zn-65	1.7E-07				○
Sr-90	1.3E-08				○
Si-32	7.9E-09				○
H-3	1.8E-09				○

20.3.3 Results of Sensitivity Analyses

Sensitivity analyses were conducted for several selected nuclides in Zircaloy-2, SUS304 stainless steel, and INCONEL alloy. Analyses in Zircaloy-4 were skipped because the sensitivity coefficients were thought to be almost the same as that in Zircaloy-2 because calculation conditions were similar. For SUS304 stainless steel, activations using the cross-section library of void ratio 0 % were evaluated because the concentrations in the case of void ratio 0 % were larger than that of void ratio 70 %.

The sensitivity coefficients of initial compositions are shown in Table 20.7. As defined in Eq. (20.1), the value shows the relative amount of variation in concentration of the target nuclide when the initial composition of element varies by a unit amount. Therefore, the source elements leading to the generation of target nuclides was clarified from the results. For example, Table 20.7a shows that Fe-55 is generated from both iron and nickel and that the contribution from iron is dominant. The results can also be useful in the evaluation of the error propagated from the measurement uncertainty of initial composition.

As defined in Eq. (20.2), a sensitivity coefficient of a cross section shows the relative amount of variation in the concentration of the target nuclide when the

Table 20.7 Sensitivity coefficients of initial composition

	Target nuclide																
	Zr-93	Ni-59	Ni-63	Co-60	C-14	Nb-94	Sb-125	Ca-41	K-40	Fe-55	Tc-99	Mo-93	Be-10	Mn-54	Ag-108 m	H-3	Zn-65
(a) Zircaloy-2																	
H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.9995	0
B	0	0	0	0	0	0	0	0	0	0	0	0	0.0334	0	0	0	0
C	0	0	0	0	5E-05	0	0	0	0	0	0	0	0.9666	0	0	0	0
N	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0	0.0003	0
Mg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Al	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Si	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ca	0	0	0	0	0	0	0	1.0000	1.0000	0	0	0	0	0	0	0	0
Ti	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mn	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0032	0	0	0
Fe	0	0	0	0.0004	0	0	0	0	0	0.9564	0	0	0	0.9967	0	0	0
Co	0	0	0	0.9980	0	0	0	0	0	0	0	0	0	0	0	0	0
Ni	0	1.0000	0.9904	0.0015	0	0	0	0	0	0.0436	0	0	0	0	0	0	0.0001
Cu	0	0	0.0096	0.0001	0	0	0	0	0	0	0	0	0	0	0	0	0.9999
Zr	1.0000	0	0	0	0	0.0001	0	0	0	0	0.0289	0	0	0	0	0	0
Mo	0	0	0	0	0	0.0001	0	0	0	0	0.9711	1.0000	0	0	0	0	0
Nb	0	0	0	0	0	0.9998	0	0	0	0	0	0	0	0	0	0	0
Cd	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.0000	0	0
Sn	0	0	0	0	0	0	1.0000	0	0	0	0	0	0	0	0	0	0
Hf	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
W	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

(b) SUS304 stainless steel

	Target nuclide							
	Ni-59	Ni-63	Fe-55	Co-60	Mn-54	Be-10	C-14	Cl-36
C	0	0	0	0	0	1.0000	1.0000	0
Si	0	0	0	0	0	0	0	0
P	0	0	0	0	0	0	0	0
S	0	0	0	0	0	0	0	1.0000
Cr	0	0	0	0	0	0	0	0
Mn	0	0	0	0	0.0027	0	0	0
Fe	0	0	0.9890	0.0819	0.9974	0	0	0
Ni	1.0000	1.0000	0.0110	0.9181	0	0	0	0

(c) INCONEL alloy 718

	Target nuclide															
	Ni-59	Ni-63	Co-60	Nb-94	Mo-93	Tc-99	Fe-55	Zr-93	Mn-54	Be-10	Cl-36	C-14	Zn-65	Sr-90	Si-32	H-3
B	0	0	0	0	0	0	0	0	0	0.5830	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0.4170	0	1.0000	0	0	0	0
Al	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0012
Si	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.7059	0.0011
P	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.2926	0.0002
S	0	0	0	0	0	0	0	0	0	0	1.0000	0	0	0	0.0015	0.0005
Ti	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0007
Cr	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0121
Mn	0	0	0	0	0	0	0	0	0.0019	0	0	0	0	0	0	0.0001
Fe	0	0	0.0001	0	0	0	0.7411	0	0.9982	0	0	0	0	0	0	0.0258
Co	0	0	0.9970	0	0	0	0	0	0	0	0	0	0	0	0	0.0004
Ni	1.0000	0.9994	0.0028	0	0	0	0.2589	0	0	0	0	0	0.0014	0	0	0.9557
Cu	0	0.0006	0	0	0	0	0	0	0	0	0	0	0.9985	0	0	0.0012
Nb	0	0	0	0.9999	0	0	0	0.9839	0	0	0	0	0	0.9841	0	0.0003
Mo	0	0	0	0.0001	1.0000	1.0000	0	0.0161	0	0	0	0	0	0.0159	0	0.0008

Table 20.8 Sensitivity coefficients of cross sections

Target nuclide	Sensitivity coefficient of cross section								
	First largest			Second largest			Others		
(a) Zircaloy-2									
Zr-93	Zr-92	(*n*, γ)	0.98	Zr-94	(*n*, 2*n*)	0.02			
Ni-59	Ni-58	(*n*, γ)	0.99						
Ni-63	Ni-62	(*n*, γ)	0.97						
Co-60	Co-59	$(n, \gamma)_m$	0.46	Co-59	(*n*, γ)	0.42			
C-14	N-14	(*n*, *p*)	1.00						
Nb-94	Nb-93	(*n*, γ)	1.00						
Sb-125	Sn-124	(*n*, γ)	0.56	Sn-124	$(n, \gamma)_m$	0.48			
Ca-41	Ca-40	(*n*, γ)	1.00						
K-40	Ca-40	(*n*, *p*)	1.00						
Fe-55	Fe-54	(*n*, γ)	0.95	Ni-58	(*n*, α)	0.04			
Tc-99	Mo-98	(*n*, γ)	1.00	Mo-97	(*n*, γ)	0.03	Zr-96	(*n*, γ)	0.03
Mo-93	Mo-92	(*n*, γ)	0.99						
Be-10	C-13	(*n*, α)	0.97	B-10	(*n*, *p*)	0.03			
Mn-54	Fe-54	(*n*, *p*)	1.00						
Ag-108 m	Cd-106	(*n*, γ)	1.00	Ag-107	$(n, \gamma)_m$	0.97			
H-3	H-2	(*n*, γ)	1.00	H-1	(*n*, γ)	0.78	He-3	(*n*, *p*)	0.01
Zn-65	Zn-64	(*n*, γ)	1.00	Cu-63	(*n*, γ)	1.00			
(b) SUS304 stainless steel									
Ni-59	Ni-58	(*n*, γ)	1.00						
Ni-63	Ni-62	(*n*, γ)	1.00						
Fe-55	Fe-54	(*n*, γ)	0.99	Ni-58	(*n*, α)	0.01			
Co-60	Ni-60	(*n*, p)	0.92	Fe-58	(*n*, γ)	0.08	Co-59	(*n*, γ)	0.04
							Co-59	$(n, \gamma)_m$	0.04
Mn-54	Fe-54	(*n*, *p*)	1.00						
Be-10	C-13	(*n*, α)	1.00						
C-14	C-13	(*n*, γ)	1.00						
Cl-36	S-34	(*n*, γ)	1.00	Cl-35	(*n*, γ)	1.00			
(c) INCONEL alloy 718									
Ni-59	Ni-58	(*n*, γ)	0.99						
Ni-63	Ni-62	(*n*, γ)	0.98						
Co-60	Co-59	$(n, \gamma)_m$	0.46	Co-59	(*n*, γ)	0.42			
Nb-94	Nb-93	(*n*, γ)	1.00						
Mo-93	Mo-92	(*n*, γ)	0.99						
Tc-99	Mo-98	(*n*, γ)	1.00						
Fe-55	Fe-54	(*n*, γ)	0.74	Ni-58	(*n*, α)	0.26			
Zr-93	Nb-93	(*n*, p)	0.98	Mo-96	(*n*, α)	0.02			
Mn-54	Fe-54	(*n*, *p*)	1.00						
Be-10	B-10	(*n*, *p*)	0.58	C-13	(*n*, α)	0.42			
Cl-36	S-34	(*n*, γ)	1.00	Cl-35	(*n*, γ)	0.97			
C-14	C-13	(*n*, γ)	1.00						

(continued)

Table 20.8 (continued)

Target nuclide	Sensitivity coefficient of cross section								
	First largest			Second largest			Others		
Zn-65	Zn-64	(n, γ)	0.99	Cu-63	(n, γ)	0.99			
Sr-90	Zr-93	(n, α)	1.00	Nb-93	(n, p)	0.98			
Si-32	Si-31	(n, γ)	1.00	Si-30	(n, γ)	0.71	P-31	(n, p)	0.29
H-3	H-2	(n, γ)	1.00	H-1	(n, γ)	1.00	Ni-58	(n, p)	0.95
							He-3	(n, p)	0.01

$(n, \gamma)_m$ means the (n, γ) reaction yielding to meta-stable state

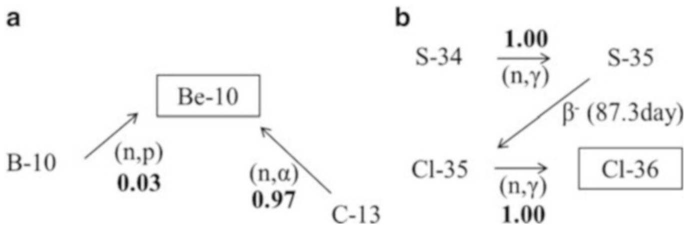

Fig. 20.2 Examples of complicated generation pathways of activation products. The values in *bold font* in the figures show the sensitivity coefficients of the cross sections. **a** Be-10 generation in Zircaloy-2. **b** Cl-36 generation in SUS304 stainless steel

cross section varies by a unit amount. Therefore, a positive value of this coefficient indicates that the target activation product is generated through the nuclear reaction. Thus, if a sensitivity coefficient is positive and large, the cross section of the nuclear reaction is significant for the generation of the target activation products. In the analyses, the objectives of reaction were six reactions treated in ORLIBJ40 library; the reaction of (n, γ), $(n, 2n)$, (n, α), and (n, p) yielding to nuclides of ground state and the reaction of (n, γ) and $(n, 2n)$ yielding to nuclides of meta-stable state. The summary of the results of sensitivity analyses of cross sections are shown in Table 20.8, where the sensitivity coefficients that are positive and more than 0.01 are extracted from all the results and listed in descending order. The results clarified the nuclear reaction dominating the generation of target nuclides. For example, it is thought that Fe-55 in Zircaloy-2 can be generated from the (n, γ) reaction of Fe-54, the (n, α) reaction of Ni-58, and the $(n, 2n)$ reaction of Fe-56. Table 20.8a clearly shows the (n, γ) reaction of Fe-54 is dominant in the generation of Fe-55.

It was remarkable that the dominant generation pathways were clarified even for the target nuclides generated through complicated pathways. Some of the examples are shown in Fig. 20.2.

Figure 20.2a shows an example of nuclides generated with some contributing pathways. Be-10 is generated in Zircaloy-2 mainly through two pathways, the (n, p) reaction of Be-10 and the (n, α) reaction of C-13. It is not predictable which pathway is dominant from the initial composition of the material. The sensitivity

Table 20.9 Initial composition of SUS304 stainless steel

Element	Value based on measurement data	Value based on the standard specification
C	–	0.08
N	0.05	–
Si	–	1.00
P	–	0.045
S	0.004	0.030
Cl	0.001	–
K	4.0E-05	–
Cr	–	19.00
Mn	–	2.00
Fe	72	68.60
Co	0.1	–
Ni	9.25	9.25
Cu	0.16	–
Zr	0.00032	–
Nb	0.02	–
Mo	0.13	–
Th	2.0E-07	–
U	2.0E-07	0.0001

coefficients clearly showed that the (n, α) reaction of C-13 is the dominant pathway for Be-10 generation in Zircaloy-2.

Figure 20.2b shows an example of nuclides generated through long and complicated generation chains. The source nuclide of Cl-36 generated in SUS304 stainless steel is ambiguous because the initial composition in this analysis does not contain chlorine, which could be the dominant source element of Cl-36. The sensitivity coefficients quantitatively clarified that S-34 is the source nuclide of Cl-36 even for the long and complicated chain.

20.3.4 Sensitivity Analysis Using the Initial Composition Based on Measured Data

The sensitivity coefficients shown in Sect. 20.3.3 are valid within the assumed analysis conditions in Sect. 20.3.1. However, the impurity elements that are not specified in the standard specification can be possibly present in the material. To know the effect of the difference in the initial composition on sensitivity coefficients, additional analyses were conducted using the initial composition based on measured data. The evaluation of activation products in SUS304 stainless steel is described here.

Table 20.10 Concentration of activation products in SUS304 stainless steel

Nuclide	Concentration of activation products (g/t)
Ni-59	4.8E + 01
Ni-63	7.8E + 00
Co-60	1.7E + 00
Fe-55	7.4E-01
C-14	1.7E-01
Cl-36	5.4E-02
Nb-94	3.4E-02
Tc-99	1.2E-02
Mo-93	1.1E-02
K-40	1.8E-04
Mn-54	1.0E-04
Zr-93	6.6E-05

Except for the initial composition, the analysis conditions described in Sect. 20.3.1 were assumed. The composition data reported by the Atomic Energy Society of Japan [6] were applied in this analysis. In this reference, the concentration distributions of some elements with their mean values and standard deviations have been determined based on several measured data. The initial composition based on measured data is shown in Table 20.9 together with that based on the standard specification.

The concentration of activation products using the initial composition based on measured data is shown in Table 20.10. As a matter of course, the concentrations were changed from those in Table 20.6b because the different initial compositions were assumed. It was found that Nb-94, Tc-99, Mo-93, K-40, and Zr-93 appeared in Table 20.10 because of the presence of niobium, molybdenum, and potassium in the initial composition. For the comparison with the sensitivity coefficients shown in Sect. 20.3.3, sensitivity analyses of cross sections were conducted for the several nuclides Ni-59, Ni-63, Fe-55, Co-60, Mn-54, C-14, and Cl-36, which were listed in both Tables 20.6b and 20.10.

The sensitivity coefficients of cross sections using the initial composition based on measured data are shown in Table 20.11. It was found that the results of Co-60, C-14, and Cl-36 are much different from those in Table 20.8b, which indicates that the dominant generation pathways of these nuclides were changed. Figure 20.3 shows the comparison of dominant generation pathways of Co-60, C-14, and Cl-36 between different analysis conditions. The source nuclides of Co-60, C-14, and Cl-36 were Co-59, N-14, and Cl-35, respectively, under the conditions based on measurement data, whereas those were Ni-60, C-13, and S-34, respectively, under the conditions based on the standard specification.

As shown in the foregoing example, the dominant generation pathway can be changed corresponding to the initial composition. The reliable measured data of initial impurity elements should be used if they are available. For any condition, sensitivity analyses on the basis of the methodology stated in this study can systematically identify the dominant generation pathways of activation products.

Table 20.11 Sensitivity coefficient of cross section in SUS304 stainless steel

Target nuclide	Sensitivity coefficient of cross section					
	First largest			Second largest		
Ni-59	Ni-58	(n, γ)	1.00			
Ni-63	Ni-62	(n, γ)	1.00			
Fe-55	Fe-54	(n, γ)	0.99	Ni-58	(n, α)	0.01
Co-60	Co-59	(n, γ)	0.46	Co-59	$(n, \gamma)_m$	0.46
Mn-54	Fe-54	(n, p)	1.00			
C-14	N-14	(n, p)	1.00			
Cl-36	Cl-35	(n, γ)	1.00			

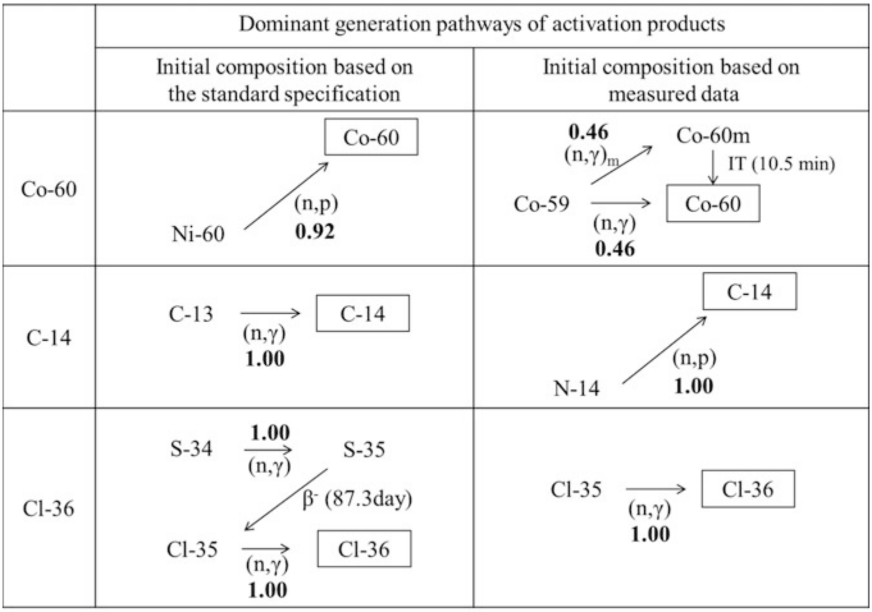

Fig. 20.3 Dominant generation pathways of activation products in SUS304 stainless steel

20.4 Conclusion

This study shows the sensitivity analyses of initial compositions and cross sections for activation products of in-core structure materials. The results clarified the source elements and nuclear reactions dominating the generation pathways of the activation products even for the nuclides generated through complicated pathways. The sensitivity coefficients of initial compositions are beneficial for the evaluation of the error propagated from the uncertainty of the initial composition of target materials. The sensitivity coefficients of cross sections are effective in selecting the objectives of nuclear reactions for the improvement of nuclear data. These results will contribute to improvement of the accuracy of numerical evaluations for the concentration of activation products.

The methodology of sensitivity analyses stated in this study is efficient for acquiring information about important impurity elements and nuclear reactions to evaluate the activation product concentrations. This methodology can be applied to the activations of ex-core structure materials if the appropriate one-group cross sections are prepared with a corresponding neutron spectrum.

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